Electronic Supplementary Material for CrystEngComm

Supplementary Information: Weak intermolecular interactions and molecular aggregation in isostructural dihaloperfluoroethanes

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Table S1. Crystal data and details of structure refinement for $BrCF_2CF_2Br$, CF_2ICF_2I and $BrCF_2CF_2I$

	$BrCF_2CF_2Br$	ICF_2CF_2I	ICF_2CF_2I	$BrCF_2CF_2I$	$BrCF_2CF_2I$	$BrCF_2CF_2I$
Pressure (GPa)	1.03(5)	0.16(5)	0.86(5)	0.60(5)	1.00(5)	3.50(5)
Temperature (K)	296(2)	296(2)	296(2)	296(2)	296(2)	296(2)
Formula weight	259.84	353.82	353.82	306.83	306.83	306.83
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$
Unit cell dimensions (Å,°) a	5.768(1)	6.563(2)	6.4133(13)	6.1357(12)	5.9698(12)	5.7683(12)
b	6.078(1)	6.293(4)	5.9350(12)	6.1449(12)	6.1503(12)	6.0823(12)
c	8.080(1)	8.935(6)	8.4792(17)	8.3967(17)	8.2360(16)	8.0112(16)
β	107.01(3)	106.47(5)	103.68(3)	108.30(3)	108.58(3)	109.92(3)
Volume ($Å^3$)	270.88(9)	353.8(3)	313.58(11)	300.57(10)	286.63(10)	264.26(9)
Z	2	2	2	2	2	2
Calculated density (g/cm^3)	3.186	3.321	3.747	3.390	3.555	3.856
Absorption coefficient (mm^{-1})	14.936	8.868	10.006	11.950	12.531	13.592
F(000)	236	308	308	272	272	272
Crystal diameter/height (mm)	0.36/0.07	0.39/0.07	0.46/0.06	0.41/0.09	0.37/0.09	0.36/0.08
θ-range for data collection (˚)	4.27 to 29.53	3.43 to 30.08	3.60 to 28.63	3.63 to 28.66	3.71 to 29.39	3.81 to 29.66
Min/max indices: h, k, l	-6/6;-7/7;-7/8	-9/9, -5/5, -10/10	-8/8, -1/1, -11/11	-8/8,-8/8,-4/4	-8/8,-7/7,-8/8	-6/6,-7/7,-10/10
Reflect. Collected/ unique (Rint)	2085/342 (0.0505)	2575/436 (0.0409)	1107/197 (0.1967)	2252/225 (0.0617)	2216/362 (0.0594)	1960/330 (0.0969)
Completeness (to θ_{max}) (%)	45.2 (to 29.53˚)	42 (to 30.08˚)	24.5 (to 28.63)	29.0 (to 28.66)	45.7 (to 29.39)	44.4 (to 29.66)
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Data/restrains/parameters	342/0/38	436/9/47	197/0/32	225/1/18	362/0/38	330/0/38
Goodness-of-fit on F^2	1.139	1.238	1.429	1.082	1.192	1.171
Final R_1/wR_2 ($I>2\sigma_1$)	0.0495/0.1138	0.0569/0.1304	0.1302/0.3029	0.1166/0.2670	0.0618/0.1153	0.0596/0.1762
R_1/wR_2 (all data)	0.0564/0.1180	0.0844/0.1446	0.1335/0.3107	0.1240/0.2734	0.0722/0.1234	0.0692/0.1991

Weighting scheme	w=1/(sigma2(Fo2)+(0.0739*P)2+0.24*P), where P=(Max(Fo2,0)+2*Fc2)/3	w=1/(sigma2(Fo2)+(0.0486*P)2+1.11*P), where P=(Max(Fo2,0)+2*Fc2)/3	w=1/(sigma2(Fo2)+(0.2000*P)2+1.11*P), where P=(Max(Fo2,0)+2*Fc2)/3	w=1/(σ2(Fo2)+(0.1087*P)2+12*P), where P=(Max(Fo2,0)+2*Fc2)/3	w=1/(σ2(Fo2)+(0.0455*P)2+2.48*P), where P=(Max(Fo2,0)+2*Fc2)/3	w=1/(σ2(Fo2)+(0.1199*P)2+2.30*P), where P=(Max(Fo2,0)+2*Fc2)/3
Largest diff. peak and hole (e.Å^{-3})	0.322/-0.443	0.408/-0.318	1.680/-1.373	0.825/-0.959	0.620/-0.575	1.438/-1.361